

5-Ethyl-1-methyl-5-(1-phenylethyl)pyrimidine-2,4,6(1H,3H,5H)-trione
61346-87-0 | DTXSID60818264

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 278 °C

Global applicability domain: Outside

Local applicability domain index: 1.70e-01

Confidence level: 6.51e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Diphenylurea

Measured: 262

Predicted: 269

[Image not found](#)

Carbaryl

Measured: 315

Predicted: 297

[Image not found](#)

N-(4-Bromophenyl)urea

Measured: 260

Predicted: 256

[Image not found](#)

Carbamic acid, phenyl-, ethyl ester

Measured: 238

Predicted: 260

[Image not found](#)

Benzoic acid, 2-phenylhydrazide

Measured: 314

Predicted: 306